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# Simulation of Pesticide Fate and Transport in Drainage Channels

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**Abstract**

Contamination in the drainage channels and creeks with pesticides used in agriculture is of a major concern in many countries. In this study the stream pesticide model RIVWQ (chemical transport model for riverine environments) was assessed for its applicability in simulating pesticide fate in drainage channels. The model was successfully calibrated against field data collected on flows and pesticide concentrations for a drainage channel from a small catchment in the Murrumbidgee Irrigation Area of southwestern New South Wales. The effects of different pesticide loading scenarios from farm fields on channel water quality were analysed by the calibrated model. The model simulated the flow rates and the pesticide concentrations in the drainage channel well. The results of the model simulation suggest that the RIVWQ model can be effectively used for predicting pesticide fate in the drainage channels and exposure assessment of pesticide in the agricultural environment.

*Keywords : RIVWQ, Model, Pesticide, Management, Drainage channel, Molinate*

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## I. Introduction

Drainage water from irrigated agriculture frequently contains mixture of pesticides. The environmental fate of pesticides is governed by complex interaction of many factors including the pesticide properties, the agronomic practices, the soil and hydrological conditions, and the weather conditions at the time of and following the pesticide application.

Bowmer et al. (1994) showed that pesticides used in irrigated agriculture in the Murrumbidgee Irrigation Area (MIA) of NSW, Australia, were presented in drainage waters at concentrations often exceeding water quality guidelines. Toxicity of these chemicals to the aquatic life is of a major concern.

The large variability in biophysical and management conditions makes it very difficult to produce definitive guidelines. The experimental resources required to monitor a broad range of

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conditions are unavailable. As such the use of models to simulate varying biophysical and management conditions is useful in obtaining a broader spectrum of results that can be used to develop management guidelines.

Model selection is important to simulate the pesticide fate in the environment. Few pesticide water quality models are available for the river system such as EXAMSII (exposure analysis modeling system) and WASP-5 (water quality analysis simulation program). EXAMSII is unable to simulate time-varying discharges and mass loadings along the channel system, while WASP-5 requires substantially more labour, computer time and disk storage.

A less detailed model developed in USA for pesticide fate simulation in tributary systems is RIVWQ (Williams *et al.*, 2004b). RIVWQ (chemical transport model for riverine environments) is more efficient in data setup, computation and file management. RIVWQ has been validated for northern Italy where it simulated stream flow processes adequately (Miao *et al.*, 2003). It was also successfully used for diazinon exposure assessment in the Sacramento river basin's main drainage canal (Snyder and Williams, 2004). RIVWQ model could be used in conjunction with surface runoff models to simulate the effects of land use, water management and pesticide management. However, observed field data are rare to use, therefore, the effects of rice crop area on molinate concentrations in the drainage channel were investigated in this study. The objective of this study was to assess the river pesticide model RIVWQ version 2.02 for its applicability in simulating the pesticide fate in drainage channels in southeast Australia.

## Ⅱ. RIVWQ Model

RIVWQ was developed by Waterborne Environmental Inc. in 1999 to address the main pesticide dissipation pathways in streams whilst minimising input requirements. RIVWQ simulates the transport of organic chemicals in tributary stream systems based on the theory of constituent mass balance. Stream system geometry is represented using a link-node approach in which the prototype is divided into a number of discrete volumes (nodes or junctions) connected by flow channels (links). The model was written to be compatible with the pesticide runoff models PRZM (pesticide root zone model), RICEWQ (pesticide runoff model for rice crops), and GLEAMS (groundwater loading effects of agricultural management systems), which operate on a daily time step.

Model inputs are provided through three files; a parameter file, a hydrology file and a chemical mass or concentration file. The model outputs include stream flow rate and chemical concentrations in water and sediment at selected nodes on daily basis.

### 1. Water balance

Water balance algorithm in RIVWQ uses storage account method. The water balance equation in each node is given by Eq. (1).

$$O = \sum I + \frac{\partial S}{\partial t} \qquad (1)$$

where, $O$ is outflow, $I$ is inflow, $S$ is storage of water in the control volume, and $t$ is time. Inflow sources include upstream flows from all connecting links and incremental discharge from external sources. The flow velocity can be calculated by either geometric rating curves or Manning's equation. The model includes the Muskingum flood routing option. For relatively long channel length the Muskingum flood routing option should be selected to take care of the travelling time along the channel. A detailed description can be found in Williams *et al.* (2004b).

## 2. Pesticide fate

The model tracks the total mass of chemical residues in the tributary stream systems from the loading points. The mass balance is calculated along each link of the node defined by users and governing equation applied to a control volume takes the following general form.

$$V\frac{\partial c}{\partial t}=\sum_{i=1}^{NC}(Q\bullet c)+\sum_{i=1}^{NC}(E_L\bullet A\frac{\partial c}{\partial x})+\Delta s \quad \cdots\cdots\cdots (2)$$

where, $V$ is the nodal volume of a stream segment, $c$ is pesticide concentration, $t$ is time, $i$ is the counter for links entering a node, $NC$ is the number of links or channels entering a node, $Q$ is the flow in a link, $E_L$ is the dispersion coefficient, $A$ is the link cross-sectional area, $x$ is longitudinal distance, and $\Delta s$ is the rate of net addition of the pesticide mass due to external input or internal transformation processes.

Within each nodal volume, RIVWQ simulates transformation processes and simultaneously tracks the mass balance of each chemical in two media: the stream water column and benthic sediments. Chemical residue in the water is assumed to be instantaneously diluted in each control volume. The pesticide mass balance equation in the water column can be expressed by:

$$\frac{\partial Mw}{\partial t}=M_{load}+M_{inflow}-Mw_{deg}+Mw_{tran}-M_{volat}$$
$$-M_{out}-M_{bed}-M_{setl}+M_{resus}\pm M_{difus} \quad \cdots (2)$$

where, $M_w$ is pesticide mass in the water, $M$ is pesticide mass, $t$ is time, *inflow* is advective flux entering the control volume along upstream links, *out* is advective flux into the downstream link, *deg* is degradation, *tran* is metabolite mass formed by transformation of the parent compound, *volat* is volatilisation, *bed* is bed sediment, *setl* is particulate settling, *resus* is resuspension, and *difus* is diffusion between the water and sediment, respectively.

Chemical partitioning between the water column and bed sediment occurs by diffusion, settling of chemical sorbed to suspended sediment, and resuspension of sorbed sediment.

The pesticide mass entering a node is either volatilised, degraded (hydrolysis, photolysis, metabolism), partitioned to sediment or lost to the downstream node. Pesticide partitioning to sediment occurs by direct partitioning, diffusion and settling of chemical sorbed to suspended sediment. These processes are represented simplistically governed by rate terms input by the user. The model can track both parent and metabolite chemicals. A detailed description can be found in Williams *et al.* (2004b).

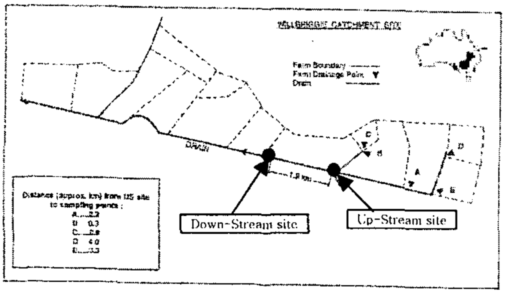

Fig. 1 Layout of the study area (Dark lines represent drainage channel and triangles represent farm drainage outlets)

## Ⅲ. Model calibration

### 1. Field data

The model was calibrated against field data collected by Thomas *et al.* (1998). They monitored drainage water at the beginning of the irrigation season 16 October to 9 December, 1993 in a small catchment in the Murrumbidgee Irrigation Area, NSW, Australia (Fig. 1). The catchment had 5 farms with a total area of 900 ha, of which 420 ha was planted to rice, 100 ha maize, 40 ha soybean, and the rest fallow. Pesticides used during the study period include molinate for rice and atrazine for maize among others. Daily composite samples were taken at two locations in the drainage channel, upstream and downstream sites 1.9 km apart. Between these two points no external inflow existed.

### 2. Calibration

In the calibration, both flow rates and pesticide concentrations should be considered. The observed flow rates and pesticide concentrations at the upstream and downstream point (1.9 km below) were used in the calibration. The input values were flow rates and chemical concentrations at the upstream point. Calibration was undertaken to fit the modeled downstream flow rates and pesticide concentrations to the observed values.

In the flow rate calibration, Manning's equation and Muskingum flood routing option were used. For drainage channels Muskingum x coefficient can be assumed to be 0.2 and Muskingum k coefficient can be estimated by dividing the length of channel reach by an assumed flow velocity (Miao et al., 2003). Channel geometry was obtained from the field survey and Manning's roughness coefficient was obtained from the reference (Chow, 1959). The daily flow rates were measured only at the upstream site.

Molinate was selected for model calibration process. Molinate is a thiocarbamate selective herbicide broadly used for control of germinating broad-leaved and grass weeds in rice farms. Its molecular formula is $C_9H_{17}NOS$. It is applied either before planting to water-seeded or shallow soil-seeded rice or post-flood, post-emergence in other types of rice culture.

For ecotoxicology of molinate, LC50 (96 h) for rainbow trout is 1.3 mg/L, bluegill sunfish 29 mg/L and goldfish 30 mg/L.

For pesticide calibration several parameter values were taken from field data, literature, and general knowledge and the others were calibrated. The volatilization coefficient, solubility and degradation rate for molinate were obtained from previous studies using RICEWQ model (Christen et al., 2005; Chung et al., 2005).

The comparison of observed upstream and modeled downstream flow rates is shown in Fig.

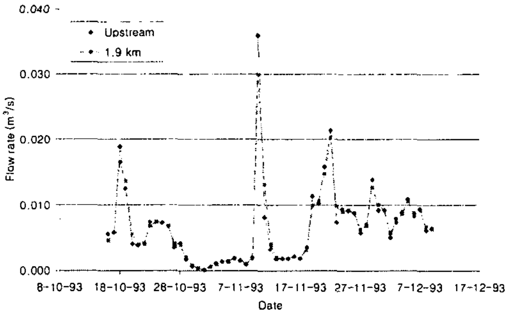

**Fig. 2 Observed upstream flow rate and model predicted downstream flow rate**

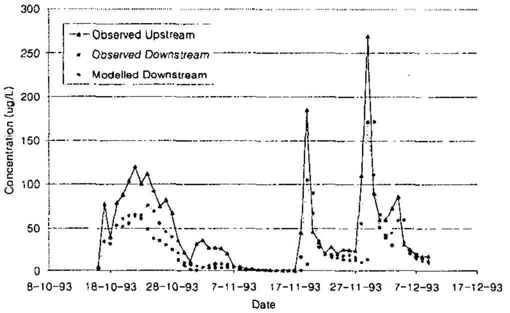

**Fig. 3 Comparison of the model simulated and observed molinate concentration**

2. This figure looks very reasonable since they are only 1.9 km apart and there was no lateral inflow in this reach. The comparison of modeled and measured flow rates at the downstream is not possible because flow rates were measured only at the upstream point.

The comparison of the observed and modeled pesticide concentrations for molinate is shown in Fig. 3. The concentrations at the upstream point were also presented for reference. In general, the model predicted downstream chemical concentrations reasonably well.

## Ⅳ. Model simulation

Drainage channel and stream water quality in agricultural area is directly related to the land use and water and pesticide management practices. Molinate concentration variations with different management practice were simulated in this study (Table 1). The same farm field used in the model calibration was used in model simulation.

With the calibrated RIVWQ model simulations were performed and the flow rates and molinate concentrations at 1.9 km and 12 km downstream points were analysed. Below the 1.9 km downstream point no external inflow was assumed and at 12 km downstream point no field measurements were made. The selection of 12 km downstream point is based upon that many water quality licence sites are about 10 km downstream of main drainage channel from the farm area boundary before entering creeks or streams.

At first, the observed values were used to simulate the flow rates and molinate concentrations at downstream points (scenario A in Table 1). Fig. 4 shows the comparison of flow rates along the channel. Flow rates at the 1.9 km downstream were very close to upstream flow rates, while those at the 12 km downstream were spread out along the time and smaller peaks with one day tame lag. The modeled flow rates look quite reasonable though no observed data were

**Table 1 Scenarios for simulating molinate concentration in the channel**

| Scenario | Rice area | Flow rate ratio at upstream | Pesticide loading ratio at upstream | Remarks |
|---|---|---|---|---|
| A | 420 ha | 1.0 | 1.0 | observed |
| B | 420 ha | 1.0 | 0.5 | 50 % loading |
| C | 210 ha | 0.76 | 0.5 | 50 % loading<br>76 % flow |
| D | 105 ha | 0.64 | 0.25 | 25 % loading<br>64 % flow |

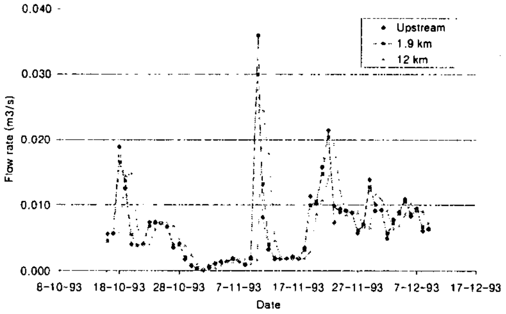

Fig. 4 Comparison of flow rates along the channel with observed rice area (upstream values are observed and the rest are simulated)

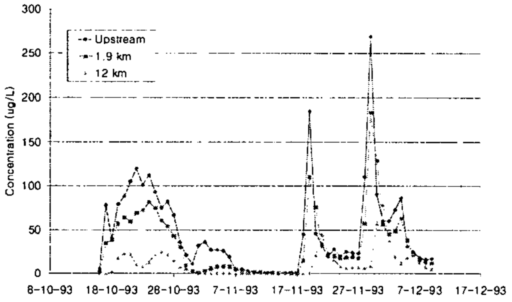

Fig. 5 Comparison of molinate concentrations along the channel with observed rice area (upstream values are observed and the rest are simulated)

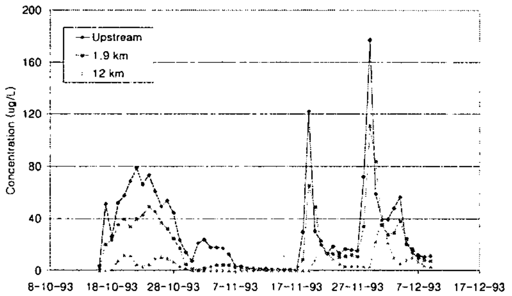

Fig. 6 Modeled molinate concentrations with a 50 % reduced pesticide loading (scenario B)

available for comparison.

Fig. 5 shows the comparison of molinate concentrations along the channel. Molinate concentrations at the 1.9 km and 12 km downstream were well represented. The molinate was dissipated mostly due to the volatilisation at the 12 km downstream..

Next, molinate loading at the upstream point were reduced by 50 % (scenario B). The concentration changes at downstream points in this case were compared with the observed values. In scenario B, the flow rates remained unchanged. Fig. 6 shows molinate concentrations in the drainage channel for the scenario B. Comparing Fig. 6 with Fig. 5 the pattern of concentration variations at three points resembles each other, but with about 50 % reduced values in scenario B. This explains the linearity between the loading and concentration with the same flow rates. The dissipation of molinate along the channel reach is well represented in Fig. 6. Also, the concentrations at the 12 km downstream point show the time lag for the traveling time well.

Next, the land area planted to rice crop was varied to see the impact of crop area on the molinate concentrations in channel. Both the flow rate and pesticide loading were changed as the rice area changed since rice paddy produces more surface drainage water with pesticide. The surface water flow rate from the rice paddy was assumed 3 times larger than that of upland crops. The observed rice crop area was 420 ha out of 900 ha total field area. Scenarios C and D had rice paddy area of 210 ha (50 % of the observed) and 105 ha (25 % of the observed), respectively. The molinate concentrations in water from the upland field are assumed to be zero, since it is applied only to the rice field

Simulated flow rate change due to the change of rice area is shown (Fig. 7). Reduction of flow rates due to the reduction of rice crop area is well represented. The flow rates with a 50 % and 75 % rice crop area reduction showed linear reduction from that of the observed rice crop area.

Simulated molinate concentrations in the channel reach with different rice crop area are shown in Fig. 8, 9 and 10. Fig. 8 shows molinate concentration at the upstream point. The concentrations with the reduced rice crop area are linearly related to the molinate concentrations for observed rice area, 420 ha. The ratios of inflow molinate concentrations for 210 ha and 105 ha to those for 420 ha rice area at the upstream point were 0.66 and 0.39, respectively. Fig. 9 shows molinate concentration at the 1.9 km downstream point. They are smaller than those at the upstream point and show the effect of rice crop area changes well. Fig. 10 shows concentrations at the 12 km downstream point. The concentration variation pattern is similar to the upstream ones but with much smaller concentrations due to the pesticide dissipation along the channel reach.

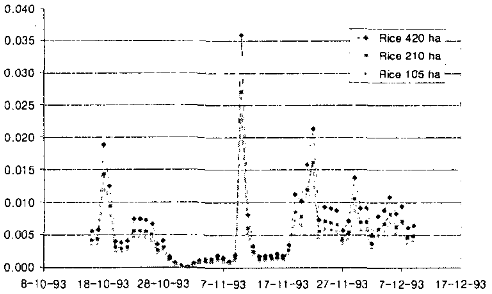

**Fig. 7** Comparison of the simulated flow rates at the upstream point with respect to rice crop area

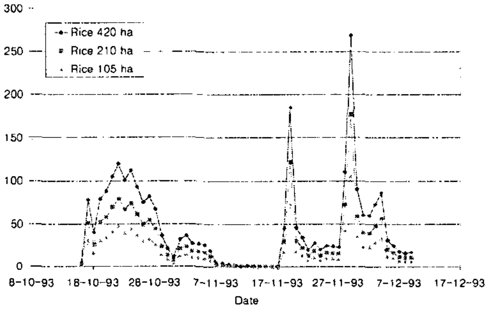

**Fig. 8** Comparison of simulated molinate concentration at the upstream point with respect to rice crop area

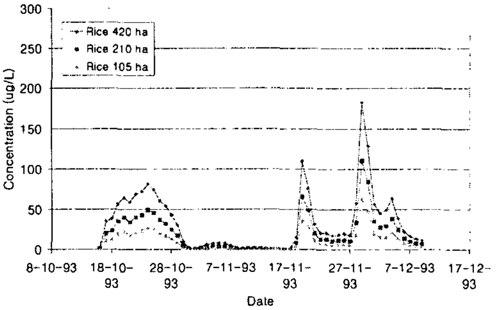

**Fig. 9** Comparison of simulated molinate concentration at the 1.9 km downstream point with respect to rice crop area

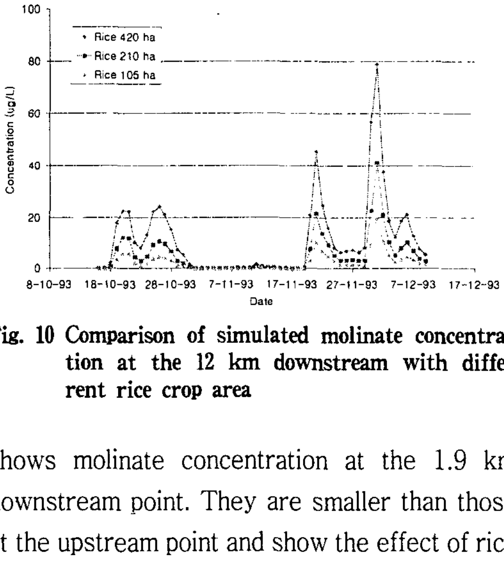

**Fig. 10** Comparison of simulated molinate concentration at the 12 km downstream with different rice crop area

## V. Summary and Conclusions

RIVWQ model is a fairly easy to use requiring limited input parameters compared to more detailed process based models. The model calibration was successful with field data, and key parameters such as decay rate, volatilisation rates and soil water partitioning coefficient were available from a previous study.

RIVWQ model was used to see the effects of rice crop area on molinate concentrations in the drainage channel in this study. Model simulated the water flow rates and molinate concentrations at the upstream point, 1.9 km and 12 km downstream points reasonably well. The results of the model simulation suggest that RIVWQ model can be effectively used for predicting pesticide fate in the drainage channels and exposure assessment of pesticide in the agricultural environment.

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